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One-dimensional Heisenberg antiferromagnet in which two $S=1/2$ and two $S=1$ spins are arranged alternatively

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Abstract

Ground-state and thermodynamic properties of the one-dimensional Heisenberg antiferromagnet in which two $S = 1/2$ and two $S = 1$ spins are arranged alternatively are studied by a quantum Monte Carlo method and by analytical estimates. It is found that the ground state of the system undergoes a second-order phase transition which accompanies the vanishing of the energy gap.

Keywords:

Ground-state phase transition; Heisenberg antiferromagnet; Mixed spin systems; One-dimensional systems; Quantum Monte Carlo simulation

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One-dimensional quantum Heisenberg antiferromagnets have been the subject of numerous studies over a long period, in particular since Haldane's prediction [1,2] of the difference between the integer-spin and half-integer-spin cases. Almost all results of these studies support the prediction, and now it is widely agreed that for isotropic nearest-neighbor (nn) exchange, the former case is massive, while the latter case is massless. Under these circumstances, the $S=1/2$ and $S=1$ alternating spin chain with isotropic nn exchange, which is a simplest example of mixed spin systems, has recently been of considerable interest both experimentally [3] and theoretically [3-7]. A characteristic feature of this chain is that it is a quantum ferrimagnet and its ground state is magnetic.

In order to explore the mixed spin chain with a nonmagnetic ground state, we discuss here the one-dimensional antiferromagnet in which two $S=1/2$ and two $S=1$ spins are arranged alternatively. We express the Hamiltonian describing the system as

$$\mathcal{H}=\sum_{\ell=1}^{N/4}\left(J_1\,\vec{s}_{4\ell-3}\cdot\vec{s}_{4\ell-2}+J_2\,\vec{s}_{4\ell-2}\cdot\vec{S}_{4\ell-1}+J_3\,\vec{S}_{4\ell-1}\cdot\vec{S}_{4\ell}+J_2\,\vec{S}_{4\ell}\cdot\vec{s}_{4\ell+1}\right), \quad (1)$$

where $\vec{s}_\ell$ ($\ell=1,\ 2,\ 5,\ 6,\ \cdots,\ N-3,\ N-2$) and $\vec{S}_\ell$ ($\ell=3,\ 4,\ 7,\ 8,\ \cdots,\ N-1,\ N$) are, respectively, the $S=1/2$ and $S=1$ spin operators, and N, being assumed to be a multiple of four, is the total number of spins. We impose periodic boundary conditions ($\vec{s}_{N+1}\equiv\vec{s}_1$). It is noted that the ground state of the system is nonmagnetic except when both J_1 and J_3 are negative.

Applying the Wigner-Eckart theorem, we may conclude that in the limit of $J_2\to\infty$ ($J_2\to-\infty$), the present system is equivalent to the $S=1/2$ ($S=3/2$) bond-alternating chain with the exchange constants $\frac{1}{9}J_1$ and $\frac{16}{9}J_3$ ($\frac{1}{9}J_1$ and $\frac{4}{9}J_3$) as far as sufficiently low energy states are concerned.

Thus, the system is gapless when $J_2 \to \infty$ and $J_1 = 16J_3 > 0$ and also when $J_2 \to \infty$ and $J_1 = 4J_3 > 0$. A perturbation calculation taking into account the lowest singlet and triplet of each unit cell ($\vec{s}_{4\ell-2}$, $\vec{S}_{4\ell-1}$, $\vec{S}_{4\ell}$, $\vec{s}_{4\ell+1}$) leads to the result that, for sufficiently small values of $|J_1|$ and $|J_2|$ with J_3 fixed at 1.0, the energy gap vanishes when $J_1 = \frac{4}{3}J_2^2 + 2J_2^3 + \cdots$.

Confining ourselves to the case where $J_1 = J_3 = 1.0$ and $J_2 > 0$, we investigated numerically the ground-state and thermodynamic properties of the system by a quantum Monte Carlo (QMC) method. Let us first discuss the ground-state properties. We carried out, at sufficiently low temperatures ($T = 0.05$ and 0.10), a QMC calculation without the global flip within the subspaces of $M \equiv \sum_{\ell=1}^{(N/4)} \left(s_{4\ell-3}^z + s_{4\ell-2}^z + S_{4\ell-1}^z + S_{4\ell}^z \right) = 0$ and 1 to estimate the energies $E(M)$ for $M = 0$ and 1, the energy gap $\Delta \equiv E(1) - E(0)$, and the nn two-spin correlation functions $\omega_{1,2} \equiv \langle s_1^z s_2^z \rangle$, $\omega_{2,3} \equiv \langle s_2^z S_3^z \rangle$, and $\omega_{3,4} \equiv \langle S_3^z S_4^z \rangle$, where $\langle \cdots \rangle$ stands for the Monte Carlo average within the $M = 0$ subspace. In the calculation, 10^6 Monte Carlo steps were performed after 10^5 initial steps for obtaining the thermal equilibrium. The Trotter number n was chosen to be $n = 12$, 16, 24, 32, 40, and 48, and the n-dependence of the QMC results was extrapolated to $n \to \infty$ by making a least-squares fit to the formula, $A_n = A_\infty + a_1/n^2 + a_2/n^4$. For both temperatures of $T = 0.05$ and $T = 0.10$, almost the same extrapolated values were obtained, and thus we consider that $T = 0.05$ is low enough to discuss the ground-state properties. The QMC calculation was carried out for $N = 8$, 16, 32, 64, and 128, for various values of J_2. As for $E(0)$, $E(1)$, and Δ for $N = 8$, we compared the extrapolated values for $T = 0.05$ with the values obtained by a method of exact diagonalization; this comparison shows that the precision in the former values goes down to the second decimal point. In order to obtain the results in the thermodynamic limit ($N \to \infty$), the

extrapolated values for the latter four N's were further extrapolated by the least-squares method using a linear function of $1/N^2$.

Fig. 1 depicts the J_2-dependence of the energy gap Δ. From this figure we see that there exists a massless point at $J_2 = J_{2\mathrm{c}} \sim 0.77$, at which the ground state of the system undergoes a second-order phase transition. Giving a thought to the J_2-dependences of the correlation functions $\omega_{1,2}$, $\omega_{2,3}$, and $\omega_{3,4}$ depicted in Fig. 2, we may schematically represent, by means of the valence-bond-solid (VBS) picture [8,9], the ground states for $J_2 < J_{2\mathrm{c}}$ and that for $J_2 > J_{2\mathrm{c}}$ as shown in Fig. 3.

Next, we briefly discuss the thermodynamic properties. Carrying out a QMC calculation which takes the global flip into account, we calculated the temperature dependence of the magnetic susceptibility and the specific heat. We obtained the result that the susceptibility per unit cell for $J_2 = 0.77$ takes a finite value in the $T \to 0$ limit; this is consistent with the fact that the energy gap vanishes at this value of J_2. We also found that for sufficiently large values of J_2 such as $J_2 = 5.0$ and 10.0, the specific heat per unit cell versus temperature curve has a double peak; the higher-temperature peak is associated with the Schottky-type peak of the two-spin system of $S = 1/2$ and $S = 1$ spins, while the lower-temperature one is associated with the specific heat peak of an antiferromagnetic $S = 1/2$ chain with bond alternation.

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Figure Captions

Fig. 1. Plots of the $N \to \infty$ energy gap Δ versus J_2. The open circles show the QMC results, and the solid lines are guides to the eye. Note that Δ vanishes at $J_2 = J_{2c} \sim 0.77$.

Fig. 2. Plots of the $N \to \infty$ correlation functions $\omega_{1,2}$ (open circles), $\omega_{2,3}$ (open squares), and $\omega_{3,4}$ (open diamonds), versus J_2, where each function is normalized by its minimum value (note that $-1/4 \leq \omega_{1,2} \leq 1/12$, $-1/3 \leq \omega_{2,3} \leq 1/6$, and $-2/3 \leq \omega_{3,4} \leq 1/3$). The solid lines are guides to the eye.

Fig. 3. Schematic representations of the ground states for (a) $J_2 < J_{2c}$ and (b) $J_2 > J_{2c}$ by means of the VBS picture. The solid circles represent the $S = 1/2$ spins, and two $S = 1/2$ spins connected by the solid line form a singlet pair. Each open ellipse surrounding two $S = 1/2$ represents an operation of constructing an $S = 1$ spin from these $S = 1/2$ spins by symmetrizing them.

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